A simple variational approach for an interacting Fermi trapped gas.

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Quantum states of a two-component Fermi trapped gas are described by introducing an effective trap frequency, determined via variational techniques. Closed expressions for the contribution of a contact interaction potential to the total energy and the pairing interaction are derived. They are valid for both few and large number of particles, given the discrete nature of the formulation, and therefore richer than the continuous expressions, which are perfectly matched. Pairing energies within a shell are explicitly evaluated and its allowed values at a given energy level delimited. We show the importance of the interaction over the trap energy as the number of particles (N) grows and the temperature decreases. At zero temperature we find a polynomial dependence of the interaction energy on the Fermi energy, whose dominant term at large N corresponds with the mean field approximation result. In addition, the role of the strength of an attractive potential on the total energy is exhibited.

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I. INTRODUCTION

In the last years, trapped degenerate two-component Fermi atomic gases have received great interest both from the theoretical [1, 2, 3, 4, 5, 6] and the experimental [7, 8] point of view. One of the reasons is that these systems offer an ideal scenario to study pairing interactions at variable interaction strength, density and temperature. It has been recognized that atoms like ⁴⁰K and ⁶Li exhibit magnetically tunable Feshbach resonances so that the swave scattering interaction may be varied from repulsive to strongly attractive. The accessible states for a dilute gas of trapped atoms may be modeled in the zerothorder approximation as a system of noninteracting particles. The simplest theoretical approach for describing trapped Fermi atoms when the interactions are not negligible, consists in approximating the system wave function as properly symmetrized products of one-particle eigenstates of an effective harmonic oscillator, whose frequency is determined via a variational procedure. The purpose of this work is to make an study of the predictions of such an approach. In particular, we obtain closed expressions of the total interaction energy that reflect its increasing relevance as the number of particles in the system is augmented, as well as closed expressions for pairing energies of atoms within a given shell.

II. FORMALISM

Let us consider a gas of Fermi atoms of mass M with internal states $|\uparrow\rangle$ and $|\downarrow\rangle$. They are in a harmonic trap that for simplicity will be assumed to be of spherical symmetry and characterized by a frequency ω_0 . An asymmetric harmonic trap can be treated in a completely analogous way. We model the interaction between atoms

in different internal states by an effective contact potential

$$V(\vec{x}_{i\downarrow} - \vec{x}_{j\uparrow}) = \frac{4\pi\alpha_0\hbar^2}{M}\delta^{(3)}(\vec{x}_{i\downarrow} - \vec{x}_{j\uparrow}) \tag{1}$$

with α_0 the scattering length. This potential is based on scattering theory at low energies. It is inexact for at least two reasons: it takes into account neither higher partial waves nor the dependence of s-wave scattering on the momentum transfer. One consequence of the latter is that no parameters beyond the scattering length such as the effective range are included in Eq.(1). Thus, this potential is expected to be valid for low energy transfer. In fact it has proven to be useful to describe cold atoms at low densities [3] and it could also be important for intermediate densities by introducing an effective scattering length [10].

The Hamiltonian of the system is taken as

$$\hat{H} = \sum_{i} \left[\frac{\hat{p}_{i}^{2}}{2M} + \frac{1}{2} M \omega_{0}^{2} |\vec{x}_{i}|^{2} \right] + \sum_{i\downarrow,j\uparrow} V(\vec{x}_{i\downarrow} - \vec{x}_{j\uparrow}). \quad (2)$$

We are interested in obtaining approximate eigenfunctions of this Hamiltonian using the variational method. The validity of such an approach is limited by the reliability of the model Hamiltonian. As a trial wave function, we consider the product of two Slater determinants, one for each internal state. These determinants are built up by the one particle eigenfunctions of a spherical harmonic oscillator of frequency ω' and quantum numbers n_x, n_y and n_z . The value of ω' should reflect the interaction effects and in the limit of zero interaction it becomes $\omega' = \omega_0$. Notice, however, that dramatic changes in ω' with respect to ω_0 are incompatible with the assumptions supporting the use of the contact interaction potential (1).

Taking into account the results summarized in the Appendix, the expectation value of the Hamiltonian for this trial function is found to be

$$\langle \hat{H} \rangle = \hbar \omega_0 \left[\frac{\epsilon_t + \epsilon_0}{2} \left(a + \frac{1}{a} \right) + \epsilon_s a^{3/2} \right]$$
 (3)

where $a = \omega'/\omega_0$,

$$\epsilon_t = \sum_{\{n_x^{\uparrow}, n_y^{\uparrow}, n_z^{\uparrow}\}} (n_x^{\uparrow} + n_y^{\uparrow} + n_z^{\uparrow}) + \sum_{\{n_x^{\downarrow}, n_y^{\downarrow}, n_z^{\downarrow}\}} (n_x^{\downarrow} + n_y^{\downarrow} + n_z^{\downarrow}) (4 \text{decomposed}, e. g., \text{ in the form } n_x \sim (3/5)n_v \text{ and } n_y = n_z \sim 1/5n_v.$$

$$\epsilon_0 = \frac{3}{2}(N^{\uparrow} + N^{\downarrow}), \tag{3}$$

$$\epsilon_s = g \sum_{\{n_x^{\uparrow}, n_y^{\uparrow}, n_z^{\uparrow}\}} \sum_{\{n_x^{\downarrow}, n_y^{\downarrow}, n_z^{\downarrow}\}} I(n_x^{\downarrow}, n_x^{\uparrow}) I(n_y^{\downarrow}, n_y^{\uparrow}) I(n_z^{\downarrow}, n_z^{\uparrow}).$$
 (6)

with $N^{(i)}$ the number of particles in a given internal state $i, g = \frac{4\pi\alpha_0}{\sqrt{\hbar/M\omega_0}}$ the scattering length in natural units and

$$I(n,m) = \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{\min\{n,m\}} \frac{(2(m-k)-1)!!}{(2(m-k))!!} \frac{(2(n-k)-1)!!}{(2(n-k))!!} \frac{(2k)!!}{(2k)!!} \frac{(2k)!!}{M_F - n_x} \frac{M_F - n_x - n_y}{M_F - n_x - n_y} = \frac{(M_F + n_x)!}{(2k)!!} \frac{(2k)!!}{M_F - n_x} \frac{M_F - n_x - n_y}{M_F - n_x - n_y} = \frac{(M_F + n_x)!}{(2k)!!} \frac{(2k)!!}{M_F - n_x} \frac{M_F - n_x - n_y}{M_F - n_x - n_y} = \frac{(M_F + n_x)!}{M_F - n_x} \frac{M_F - n_x - n_y}{M_F - n_x} \frac{M_F - n_x}{M_F - n_x} \frac{M_F$$

 ϵ_t , ϵ_0 and ϵ_s can be identified with the trap, zero point and interaction energies in units of $\hbar\omega_0$, respectively. Taking a as a variational parameter, the condition that the expectation value of the Hamiltonian becomes an extremum reduces to

$$a^5 - \frac{1}{9} \left(\frac{\epsilon_t + \epsilon_0}{\epsilon_s}\right)^2 (a^2 - 1)^2 = 0. \tag{8}$$

If the scattering length is negative, in order to admit a variational solution corresponding to a minimum of the energy it is necessary that

$$a^{5/2} < -\frac{4(\epsilon_t + \epsilon_0)}{3\epsilon_s}. (9)$$

Once the proper value of the variational parameter has been determined, the properties of the system can be estimated. In particular, the pairing energy between two particles of quantum numbers n^{\uparrow} , n^{\downarrow} whose wave functions are $\phi_{n^{\uparrow}}(\vec{x})$ and $\phi_{n^{\downarrow}}(\vec{x})$ is given by

$$\langle V \rangle = \int d^3x \phi_{n\uparrow}^*(\vec{x}) \phi_{n\uparrow}(\vec{x}) \phi_{n\downarrow}^*(\vec{x}) \phi_{n\downarrow}(\vec{x}) \qquad (10)$$
$$= \frac{4\pi\alpha_0}{\sqrt{\hbar/M\omega'}} I(n_x^{\downarrow}, n_x^{\uparrow}) I(n_y^{\downarrow}, n_y^{\uparrow}) I(n_z^{\downarrow}, n_z^{\uparrow}).$$

For atoms in a trap with effective frequency ω' , an energy level $\epsilon_{n_v} = \hbar \omega' (n_v + 3/2)$ exhibits a degeneracy $(n_v + 2)(n_v + 1)/2$ arising from the condition $n_x + n_y + n_z = n_v$. Then the pairing energy between two particles in the same shell is directly given by the restriction $n_v^{\uparrow} = n_x^{\uparrow} + n_y^{\uparrow} + n_z^{\uparrow} = n_x^{\downarrow} + n_y^{\downarrow} + n_z^{\downarrow} = n_v^{\downarrow}$. In order to illustrate the pairing energy features, let us explore the behavior of the universal dimensionless quantity

For a given quantum number n, the integrals I(n,m) achieve its maximum value for n=m. In Figure 1, we plot the allowed region of the δ_{n_v} values, delimited by solid line curves. They correspond to its maximum δ_{max} (top) and minimum δ_{min} (bottom) values, for $0 < n_v < 200$. Systematically δ_{max} corresponds to two quantum numbers equal to zero, for instance, $n_y = 0$, $n_z = 0$, while $n_x = n_v$. Meanwhile δ_{min} is achieved when n_v is decomposed, e. g., in the form $n_x \sim (3/5)n_v$ and $n_y = n_z \sim 1/5n_v$.

III. GROUND STATE.

As a particular application of these formulae we consider the ground state wave function corresponding to a configuration where all the possible states up to the non interacting Fermi energy $\epsilon_F = \hbar\omega_0(\mathcal{M}_F + 3/2)$ are occupied. To characterize the system under these conditions, we need to calculate the symmations

$$\sum_{n_x=0}^{(2k)M_F} \sum_{n_y=0}^{M_F-n_x} \sum_{n_z=0}^{M_F-n_x-n_y} 1 = \frac{(\mathcal{M}_F+1)^3 + 3(\mathcal{M}_F+1)^2 + 2(\mathcal{M}_F+1)^2}{6}$$

$$\sum_{n_x=0}^{\mathcal{M}_F} \sum_{n_y=0}^{\mathcal{M}_F - n_x} \sum_{n_z=0}^{\mathcal{M}_F - n_x - n_y} n_x = \frac{(\mathcal{M}_F + 1)^4 + 2(\mathcal{M}_F + 1)^3 - (\mathcal{M}_F + 1)^3}{24}$$

The first sum let us evaluate the number of particles $N^{(i)}$ for such a configuration in terms of the Fermi energy. While the second gives one third of the corresponding trap energy $\epsilon_t^{(i)}$, in $\hbar\omega_0$ units, neglecting the zero point energy. Notice that for large $\mathcal{M}_{\mathcal{F}}$ the trap energy becomes

$$\epsilon_t^{(i)} = \frac{3}{4} N^{(i)} \mathcal{M}_{\mathcal{F}} = \frac{3}{4} N^{(i)} \left[\frac{\epsilon_F}{\hbar \omega_0} - \frac{3}{2} \right].$$
 (14)

That is, the discrete summation relation between these variables coincides with that obtained in the standard procedure that works with an approximate continuum spectra. In Table I, the behavior of the dimensionless quantities $N^{(i)} = N^{\uparrow} = N^{\downarrow}$, $\epsilon_t^{(i)}$ and $\tilde{\epsilon}_s = \epsilon_s/g$ as a function of \mathcal{M}_F is illustrated. Notice the increasing relevance of the interaction term $\tilde{\epsilon}_s$ compared to the ϵ_t . While at $\mathcal{M}_{\mathcal{F}} = 10$ it represents only a 13.6%, at $\mathcal{M}_{\mathcal{F}} = 300$ it becomes 47% as big as ϵ_t . In fact, for $0 < \mathcal{M}_F \sim 200$, we have found that $\tilde{\epsilon}_s$ has a polynomial behavior of the form

$$\tilde{\epsilon}_s = (2\pi)^{-3/2} + \mathcal{M}_F^{1/2} (c_0 + c_1 \mathcal{M}_F + c_2 \mathcal{M}_F^2 + c_3 \mathcal{M}_F^3 + c_4 \mathcal{M}_F^4)$$
(15)

with

$$c_0 = 0.11671733,$$
 $c_1 = 0.18747855,$ $c_2 = 0.12399665,$ $c_3 = 0.03706759,$ $c_4 = 0.00411862$

 $\delta_{n_v}(n_x, n_y, n_z) = I(n_x, n_x)I(n_y, n_y)I(n_z, n_z), \qquad n_x + n_y + n_z \text{with} \text{na.relative error of the order of } 10^{-7} \text{ for } \mathcal{M}_F > 40 \text{ and}$ $(11) \qquad \text{of order less or equal to } 10^{-4} \text{ for } \mathcal{M}_F < 40. \text{ That is, our}$

numerical calculations show that the interaction energy scales as $\mathcal{M}_F^{4.5}$ for large \mathcal{M}_F growing faster than $\epsilon_t \sim \mathcal{M}_F^4$. This numerical result can be understood within the mean field approximation as follows:

In general, for a given mixture of Fermi atoms described by the product of two Slater determinants formed by one-particle eigenfunctions $\phi_a^{(i)}(\vec{r_j})$ of an effective one particle Hamiltonian, $\hat{h} = \hat{p}^2/2M + v(\vec{r})$, the expectation value of a contact interaction potential is determined by

$$\sum_{i^{\downarrow},j^{\uparrow}} \langle \delta(\vec{x}_{i^{\downarrow}} - \vec{x}_{j^{\uparrow}}) \rangle = \sum_{n^{\uparrow},n^{\downarrow}} \int d^{3}x \phi_{n^{\uparrow}}^{*}(\vec{x}) \phi_{n^{\uparrow}}(\vec{x}) \phi_{n^{\downarrow}}^{*}(\vec{x}) \phi_{n}(\mathbf{16})$$

$$= \int d^{3}x \rho^{\uparrow}(\vec{x}) \rho^{\downarrow}(\vec{x})$$
(17)

where $\rho^{(i)}(\vec{x})$ represents the spatial density of atoms of *i*-type. In our problem, the one particle Hamiltonian is that of a spherical harmonic oscillator of frequency ω' . Then, at zero temperature and for a large number of atoms, the Thomas-Fermi approximation leads to the expression [1, 2]

$$\rho^{(i)}(\vec{x})_{T=0} \sim \frac{N^{(i)}}{R_F^3} \frac{8}{\pi^2} \left[1 - \frac{r^2}{R_F^2} \right]^{3/2}, \qquad R_F = \left[\frac{2\epsilon_F}{M\omega'^2} \right]^{1/2}.$$
(18)

So that.

$$\frac{4\pi\alpha_0\hbar^2}{M} \sum_{i^{\downarrow},j^{\uparrow}} \langle |\delta(\vec{x}_{i^{\downarrow}} - \vec{x}_{j^{\uparrow}})| \rangle \sim g\hbar\omega' \frac{512}{\sqrt{2}\pi^3 2835} \left[\frac{\epsilon_F}{\hbar\omega'} \right]^{4.5} (19)$$

 $\sim 0.004118625 \ g\hbar\omega_0 a^{3/2} \mathcal{N}_{2}$

Eq. (15) is consistent with the later result and, in fact, generalizes this formula for small \mathcal{M}_F .

Another useful result to exploit the variational approach, for large $N^{(\uparrow)} = N^{(\downarrow)} = N^{(i)}$, is that the variational equation (8) can be approximated by

$$0.419372q\tilde{R}_F a^5 - (a^2 - 1)^2 = 0, (21)$$

where $\tilde{R}_F = R_F / \sqrt{\hbar/M\omega'} = (48N^{(i)})^{1/6}$ is the characteristic size of the trapped degenerate Fermi gas in the natural units of the trap. In Table II, the results of the variational calculation are exemplified for $\mathcal{M}_F = 150$, corresponding to about half a million atoms of a given internal state. An attractive interaction is considered and the corresponding coupling constant q is varied, leading to optimal values of a via the variational equation. Notice that the information about the trap parameter (ω_0) and the atom characteristics (M and α_0) are contained in g. Therefore the results are not restricted to neither a specific atom nor trap. In this table, the exact expectation values of the Hamiltonian in $\hbar\omega_0$ units divided by the total number of particles $N = N^{\uparrow} + N^{\downarrow}$ are shown for $\omega' = \omega_0$ ($\langle \tilde{E} \rangle_{\omega' = \omega_0}$) and for an optimized choosing of the variational parameter a ($\langle \tilde{E} \rangle_{min}$). As predicted by Eq. (9) no minima can be found for |q| > 0.9. In this case the expectation value of the energy exhibits a maximum

TABLE I: Behavior of the dimensionless quantities: number of particles N, trap energy ϵ_t and interaction energy $\tilde{\epsilon}_s = \epsilon_s/g$ as a function of \mathcal{M}_F .

Ī	\mathcal{M}_F	$N^{(i)}$	$\epsilon_t^{(i)}$	$ ilde{\epsilon}_s$
ſ	5	56	210	25.4
Ī	10	286	2145	293.0
Ī	20	1771	26565	4512.3
Ī	30	5456	122760	24396.9
Ī	40	12341	370230	82991.0
	50	23426	878475	217041.8
)	60	39711	1786995	479024.0
Ī	70	62196	3265290	938926.7
Ţ	80	91881	5512860	1685871.8
)	90	129766	8759205	2829605.9
ſ	100	176851	13263825	4501889.6
Ī	150	585276	65843550	27103302.6
Ī	300	1373701	206055150	97458248.4

at a given value of a < 1 and decreases monotonically for a > 1. That is, the gas would behave as trapped in a harmonic potential of arbitrarily large frequency. Therefore, it would collapse. However, this prediction is beyond the validity region of the model.

A mechanical instability of a strongly interacting Fermi gas arises when attractive interactions overcome repulsive effects such as the Fermi pressure [3]. In actual experimental realizations [10], there are mechanisms not represented by the simple model Eq.(1) that may stabilize the system. For instance, repulsive contributions to the interaction arising from higher order partial waves [11], or within the s-wave scattering scheme, effective potentials resulting from adding the ladder diagrams in a many-body perturbative approach [9]. Assuming densities that guarantee an interatomic separation larger than the range of the potential but much shorter than the scattering length, Heiselberg found that an effective s-scattering amplitude arises, which always favors the stability of a two component Fermi gas.

A mixture of spin-polarized atomic ⁶Li in two possible hyperfine states constitutes a specially interesting system [3, 8, 10]. It exhibits magnetic tunable Feshbach resonances that enable the variation of the scattering length from strongly repulsive to strongly attractive. In fact, an anomalously large and negative scattering length $\alpha_0 = -2160$ a₀ has been already measured [12]. The coupling constant corresponding to this value of α_0 , for a typical trap of mean frequency $\omega_0 \sim 3 \text{kHz}$ is g = -0.725. Then the effective frequency for half a million atoms is $\omega' = 1.48\omega_0$. It differs significantly from the trap frequency; the model potential and our variational approach are at the border of its applicability.

TABLE II: Average energy per atom for $\omega' = \omega_0$, $\langle \tilde{E} \rangle_{\omega' = \omega_0} / N^{(i)}$ and for an optimized variational parameter a, $\langle \tilde{E} \rangle_{min} / N^{(i)}$, as a function of the strength of an attractive potential, g.

g	$\langle \tilde{E} \rangle_{\omega' = \omega_0} / N^{(i)}$	a	$\langle \tilde{E} \rangle_{min} / N^{(i)}$
-0.05	111.34	1.02	111.33
-0.10	110.18	1.03	110.13
-0.20	107.87	1.07	107.63
-0.30	105.55	1.11	104.99
-0.40	103.24	1.17	103.24
-0.50	100.92	1.23	99.12
-0.60	98.61	1.32	95.79
-0.7251	95.71	1.48	91.03
-0.80	93.98	1.65	87.64
-0.85	92.82	1.90	84.93

IV. INTERACTION ENERGY FOR $T \neq 0$.

A detailed description of the behavior of the Fermi gas at finite temperature including interactions, can be given by evaluating the variational wave functions for a set of accessible quantum states and performing the proper statistical average to infer properties like average energies or densities. In this section we shall make an approximate calculation where the starting point is Eq. (16). This approach $has\ not$ a rigorous theoretical basis but should give us a reasonable estimate of the energy shift at finite temperatures. According to the Thomas-Fermi approximation, valid for a large number of particles, the atomic density for a trapped Fermi gas, at a given temperature T, is [2]

$$\rho^{(i)}(\vec{x},T) = \frac{1}{2\pi} \int \frac{d^3k}{e^{\beta[\hbar|\vec{k}|^2/2M + 1/2M\omega'^2r^2] - 2} + 1}, \quad (22)$$

where $\beta = 1/k_BT$. Defining the function

$$\mathcal{I}(\xi) = \int d\eta \int d\eta' \int d\zeta \eta^2 \eta'^2 \zeta^2 \left[e^{\eta^2 + \zeta^2 - \xi} + 1 \right]^{-1} \left[e^{\eta'^2 + \zeta^2 - \xi} + 1 \right]^{-1}$$

we can estimate the interaction energy at such temperature by generalizing equation (16) to consider temperature dependent densities:

$$\langle V(N,T)\rangle = \frac{4\pi\alpha_0\hbar^2}{M} \int d^3x \rho_{\uparrow}(\vec{x},T)\rho_{\downarrow}(\vec{x},T) \quad (24)$$
$$= \frac{4\pi\alpha_0\sqrt{M}2^{9/2}}{\pi^3\hbar^4\omega^{3/3}\beta^{9/2}} \mathcal{I}(\xi) \quad (25)$$

where the parameter $\xi = \mu \beta$ is given implicitly by

$$N^{(i)} = \frac{1}{2\hbar\omega'} \int \frac{\epsilon^2 d\epsilon}{e^{\beta(\epsilon-\mu)} + 1}$$
 (26)

with μ the chemical potential.

In Figure 2, the behavior of the dimensionless quantity $\tilde{v}(N,T) = \langle V(N,T) \rangle \sqrt{\hbar \omega' M}/(4\pi\alpha_0 N)$ as a function of

the temperature is exemplified for $N=10^5$. We can observe that although the interaction may be negligible for $k_BT > \epsilon_F$ its relevance increases dramatically for $k_BT < \epsilon_F$.

V. DISCUSSION AND CONCLUSIONS.

We have studied the role of the s—wave contact interaction between Fermi atoms in different states confined in a trap by using a simple variational approach, where the interaction effects on the variational wave function are resumed in an effective frequency. We have found closed expressions for the overlap integrals that admit a fast convergence and allow a quite direct evaluation of pairing energies and total interaction energies.

Concerning the pairing energies between atoms with the same trap energy $\epsilon_T = \hbar \omega' (n_v + 3/2)$ we determine the region of relevance: they become maximum for atoms with equal quantum numbers and in states which oscillate in a given axis with excitation number $n_i = n_v$ while remain in the minimum oscillating state in the other directions $n_j = 0$ $j \neq i$. For a spherical trap, there is no privileged axis of oscillation. Meanwhile, a direct extension of the results here obtained, shows that for a completely asymmetric trap, oscillations in the direction of the highest effective frequency exhibit a higher pairing energy. These results can be compared with those found for the isotropic trap in spherical coordinates [13]. There the individual wave functions have a well defined angular momentum l, and it is natural to consider paired state functions within a given shell n_v that are eigenfunctions of the total angular momentum L. In that case the greatest pairing energies correspond to $n_v = l$ and L = 0. These paring energies do not decrease as n_v increases. For our much simpler two-particle states, δ_{max} decreases as n_v . However, our results have a direct translation for anisotropic traps, while the relevance of angular momentum coupled states is highly dependent on the spherical operators that could permit the definition of more tightly bound two-particle states for anisotropic traps.

We have found that the contribution of the contact interaction potential to the total energy of the fermionic ground state behaves as a polynomial, Eq. 15. Being valid for both few and many atoms, this expression shows the increasing relevance of the interaction terms with respect to the trap energies as the number of particles grows. In the large N region, the variational equation to determine the effective trap frequency relates the variational parameter with the geometric factor \tilde{R}_F . Meanwhile the stability criteria (9) restricts the admissible values of the coupling constant q. Beyond this limit both the model potential and the simple trial wave function have not a clear justification. As an extension to finite temperature we elaborate on a possible form of the interaction energy expectation value and find that it becomes increasingly relevant for $k_BT < \epsilon_F$ as T diminishes.

The approximations made in this work could be valid not just for dilute gases but also for denser systems by taking α_0 as an effective scattering length. A more precise study can be made by solving the Hartree-Fock equations of the system using the contact interaction [5] or working with a different model potential and more sophisticated trial wave functions [14]. The computational load of such an approach restricts actual calculations to no more than hundreds of particles. Here, we have shown explicit results up to 10⁶ particles. The possibility of incorporating correlation effects, that is, working with more than one Slater determinant for each type of atoms as well as other forms of the effective interaction potential is under way.

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VI. APPENDIX.

In this appendix, integrals of the form

$$\mathcal{H}(n,m) = \int_{-\infty}^{\infty} d\zeta e^{-2\zeta^2} H_n^2(\zeta) H_m^2(\zeta). \tag{27}$$

with H_n the Hermite polynomials are evaluated. A closed expression of these integrals may be obtained employing the Rodrigues formula for Hermite polynomials. This leads to expressions that contain summations of terms with alternating signs. Here, we look for an expression in terms of finite fast convergent summations. To that end, consider the fact [15]

$$[H_n(\zeta)]^2 = \frac{(-1)^n}{\pi} \frac{(n!)^2 2^n}{(2n)!} \int_0^{\pi} (\cos y)^n H_{2n}(x(1-\sec y)^{1/2}).$$
(28)

Besides [16]

 $\int_{-\infty}^{\infty} e^{-px^{2}} H_{2m}(bx) H_{2n}(cx) dx = (2m)!(2n)! \sqrt{\frac{\pi}{p}} \sum_{k=0}^{\min\{n,m\}} \frac{1}{(m-k)!(n-k)!(2k)! \frac{(29)}{M\omega}} \frac{1}{\hbar} \frac{1}{\sqrt{\pi} 2^{m} m!} \mathcal{H}(n,m)$ $\cdot \left(\frac{b^{2}-p}{p}\right)^{m-k} \left(\frac{c^{2}-p}{p}\right)^{n-k} \left(\frac{2bc}{p}\right)^{2k}$ so that

$$\mathcal{H}(n,m) = \frac{(n!)^2 (m!)^2}{\pi^2} \sqrt{\frac{\pi}{2}} \sum_{k=0}^{\min\{m,n\}} \frac{(-2)^{2k}}{(m-k)!(n-k)!(2k)!} \cdot \overline{(30)} \sqrt{\frac{M\omega}{\hbar}} I(n,m).$$

$$\cdot \int_0^{\pi} dy (\cos y + 1)^{n-k} (\cos y - 1)^k \int_0^{\pi} dy' (\cos y + 1)^{m-k} (\cos y - 1)^k$$

but

$$\int_0^{\pi} dy (\cos y + 1)^{m-k} (\cos y - 1)^k = (-1)^k 2^m \int_0^{\pi} \cos^{2(m-k)} (y/2) \sin^{2k} (y/2) \sin^{2$$

$$\int_0^{\pi/2} \sin^{\mu-1} x \cos^{\nu-1} x dx = \frac{1}{2} B(\frac{\mu}{2}, \frac{\nu}{2})$$
 (32)

with B(r,s) the Bernoulli numbers, thus

$$\mathcal{H}(n,m) = \frac{2^{m+n}(n!)^2(m!)^2}{\pi^{3/2}\sqrt{2}} \cdot \sum_{k=0}^{\min\{m,n\}} \frac{4^k B(m-k+1/2,k+1/2)B(n-k+1/2,k+1/2)}{(m-k)!(n-k)!(2k)!}$$

Besides [15]

$$B(r,s) = \frac{\Gamma(r)\Gamma(s)}{\Gamma(r+s)}, \qquad \Gamma(n+1/2) = \frac{\sqrt{\pi}}{2^n}(2n-1)!!$$
 (34)

We can thus conclude that

$$\mathcal{H}(n,m) = n!m! \sqrt{\frac{\pi}{2}} \sum_{k=0}^{\min\{m,n\}} \frac{4^k (2m - 2k - 1)!! (2k - 1)!! (2n - 2k - 1)!}{(m - k)! (n - k)! (2k)!}$$
(35)

 $= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{M\omega}{\hbar}} \sum_{n=1}^{\min\{m,n\}} \frac{(2n-2k-1)!!}{(2n-2k)!!} \frac{(2m-2k-1)!}{(2m-2k)!!}$

and the expectation value of the one-dimensional contact interaction is then given by

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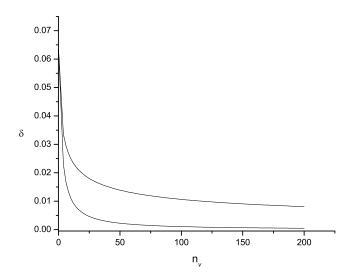


FIG. 1: Behavior of the dimensionless pairing interaction δ_{n_v} as a function of the energy level quantum number n_v . The allowed region is delimited by its maximum δ_{max} (top curve) and minimum δ_{min} (bottom curve).

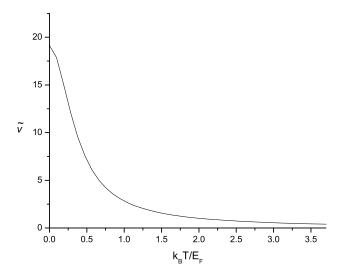


FIG. 2: Behavior of the interaction $\tilde{v}(N,T)$ for $N=10^5$ atoms as a function of the temperature.